



NANO – 2014

**3rd International Conference “Nanotechnologies”
NANO – 2014
October 20 – 24, 2014, Tbilisi, Georgia**

Welcome to Nano – 2014!
Conference is organized by the Georgian Technical University



Footbridge of Peace on the Mtkvari River, Tbilisi, Georgia

3rd International Conference “Nanotechnologies” (NANO – 2014) will be devoted the methods of synthesizing of nanomaterials, studying their structure, chemical, physical and technological properties, and applications in techniques. Conference will provide an evaluation of the present state-of-art in this field of knowledge, new achievements and prospects of developments in nanotechnologies. At the planned oral and poster sessions, it will be presented results of experimental investigations of nanosystems, as well as theoretical approaches to the modeling of such systems. Conference will be a forum of nanoscientists for broad interdisciplinary discussions and, therefore, not only intensify the actual collaboration, but also facilitate the future developments of international cooperation in nanotechnology research.

Oral and poster sessions will be devoted to:

- Obtaining of nanosystems and nanostructured materials
- Analysis of nanomaterials
- Nanophysics
- Nanochemistry
- Nanobiomedical Science
- Nanoengineering
- Nanotechnology in Industry
- Social Aspects of Nanotechnology
- Nanotechnology Education

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Paata Kervalishvili

Levan Matsaberidze

Shota Sidamonidze

Michael Vepkhvadze

Dates of Conference

Abstracts

Abstracts submission deadline :

31 March, 2014

Notification of acceptance :

30 April, 2014

Registration of Conference participants

Finishing of registration :

31 August, 2014

Attention: Registration Fee for all the participants, who is the (co)author of a presentation included in the Conference Program, will be paid by the Conference Organizer – **Georgian Technical University**.

Hotel Reservations

Information on Hotels, where Conference participants will be accommodated, will be provided :

31 July, 2014

Publication of Conference Proceedings

Abstracts of all the presentations included in Conference Program will be published as a separate volume and Abstracts Book will be handed to Conference attendees.

Full-texts of the presentations made at Conference will be published in the international journal of nanosciences and nanotechnologies **Nano Studies** (www.NanoStudies.org).

Conference working language is English

Abstracts, slides for oral presentations, posters and texts of papers should be prepared in **English**. Conference participants can make their oral presentations in **Georgian** or **Russian** as well on condition that Organizing Committee is provided with text in English to ensure its simultaneous interpretation.

Social Program

There are planned:

- Welcome party for participants
- Excursion “Tbilisi by Night”
- Trip in town Mtskheta, the old capital and religious center of Georgia
- Trip in town Signaghi and Kakheti, the region of Georgian wine-making
- Gala-banquet for participants

Attention: Social program for all the participants will be made free of charge by the Conference Organizer – **Georgian Technical University**.

Contact

Participants are asked to send their personal details and abstracts to Member of the National Organizing Committee **Prof. Levan Chkhartishvili**: chkharti2003@yahoo.com.

One-page Abstracts should be prepared according to the following template (see next page).

Font – Sylfaen

Size – 11

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ON THERMAL CONDUCTIVITY OF BORON DOPED WITH METALS

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Boron of β -rhombohedral modification (β -B) doped with metals (Me) is a promising high-temperature thermoelectric [1]. The Me atoms usually fill interstitials called as A, D and E. The quasi-classical calculations focused on binding energy of Me impurities in β -B lattice and their electron levels were presented elsewhere [2].

Present work is an attempt to analyze how these impurities act as scattering centers for heat-carrying phonons reducing thermal conductivity and improving in this way the β -B's thermoelectric figure-of-merit. The vibration frequencies ω_{Me} (in cm^{-1}) for 17 dopant metals (Li, Mg, Al, Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zr, Nb, Hf, Ta and Re) have been calculated by same method.

In the β -B phonon spectrum [3], there are bands at 150 – 650 and 650 – 1050 cm^{-1} , and also the peak at 1250 cm^{-1} (indicating vibrations of the unit cell central atom). All of the calculated vibration frequencies ω_{Me} lie above these bands, within the range 1080 – 4380 cm^{-1} , and, therefore, should be attributed to localized modes. The only experimental report [4] on the localized mode identified as the vibration of Ta atoms accommodated in β -B crystal is 2200 cm^{-1} , which is well-consistent with 2260 cm^{-1} calculated for Ta localized in a D-interstitial.

More detailed comparison can be realized based on the thermal conductivity measurements. Let concentration of Me impurities equals to A_{Me} , while T is the sample's temperature. For the physical case, we can significantly simplify the expression [5] of momentum relaxation time of heat-carrying phonons scattered by localized vibrations. If the thermal conductivity κ_{Me} of doped β -B is calculated according to Matthiessen rule $\kappa_0/\kappa_{Me} \approx 1 + \hbar\omega_{Me} A_{Me} / kT \exp((\hbar\omega_{Me} - \varepsilon) / kT)$, where κ_0 is the thermal conductivity of undoped β -B determined by the cumulative effect of all mechanisms of scattering except for the scattering by localized vibrations. By solving this equation with respect to the unknown energy-parameter ε we obtain its value from measurable ones.

In most cases, ε has almost identical values, 0.5 – 0.6 eV, which can be interpreted in such a way that all of the impurities effectively scatter phonons. If the doping effects of a given Me for interstitials of any type can be described by almost the same ε , we can assume that those atoms in all possible positions act as almost identical scattering centers. The last is true for relatively light elements – V, Fe, Co, Ni and Cu – due to the proximity of frequencies. However, for heavy elements Zr and Hf accommodated in D- and E-type interstitials, we obtain lower ε : 0.2 – 0.4 eV. It should be associated with noticeable differences in frequencies of localized vibrations of heavy atoms when they are located in the interstitials of various types. Note that the thermal conductivity in Zr- and Hf-doped β -B can be explained by the same ε if we assume that these impurities are predominantly concentrated in the A-type voids. Structural studies of the samples doped with Zr and Hf indicate the high, low and middle occupancies of interstitials of type A, D and E, respectively, that is consistent with above interpretation. For the relatively light elements, particularly Fe and Cu, the occupancies are quite different: low – high – very low and low – high – high, respectively. But in such cases, the distribution of impurities between interstitials not has a significant effect on the κ_{Me} .

1. D. L. Gabunia, O. A. Tsagareishvili, L. S. Chkhartishvili, G. F. Tavadze. In: Perspective Mater. & Nanomater. 2007, Kharkov: KhPTI – Contrast, 211.
2. L. Chkhartishvili, I. Murusidze, M. Darchiashvili, O. Tsagareishvili, D. Gabunia. Solid State Sci. 14 (2012) 1673.
3. U. Kohlmann, H. Werheit, T. Dose, T. Lundström. In: Proc. 9th Int. Symp. Boron, Borides & Rel. Comp. 1987, Duisburg: UDG, 340.
4. O. A. Golikova, G. V. Tsagareishvili, M. M. Usmanova, T. Khomidov, D. L. Gabunia, A. S. Umarov, Z. Mirzazhonov. Bull. Acad. Sci. Uzb. SSR (Ser. Phys. & Math.) 5 (1981) 88.
5. B. M. Mogilevskij, A. F. Chudnovskij. Thermal Conductivity of Semiconductors. 1972, Moscow: Nauka.